1-(Pentachloroethyl)benzene

Inchi: InChI=1S/C8H5Cl5/c9-7(10,8(11,12)13)6-4-2-1-3-5-6/h1-5H
InchiKey: AXVLZOYLQOEKAO-UHFFFAOYSA-N
Formula: C8H5Cl5
SMILES: ClC(Cl)(Cl)C(Cl)(Cl)c1ccccc1
Mol. weight [g/mol]: 278.39
CAS: 706-93-4

Physical Properties

Property code	Value	Unit	Source
gf	74.92	kJ/mol	Joback Method
hf	-68.12	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	55.01	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.687		Crippen Method
mcvol	161.020	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	589.81	K	Joback Method
tc	859.44	K	Joback Method
tf	310.65 ± 2.00	K	NIST Webbook
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.85	J/mol×K	589.81	Joback Method
cpg	311.67	J/mol×K	634.75	Joback Method
cpg	320.20	J/mol×K	679.69	Joback Method
cpg	327.59	J/mol×K	724.63	Joback Method
cpg	334.02	J/mol×K	769.57	Joback Method
cpg	339.64	J/mol×K	814.51	Joback Method
cpg	344.61	J/mol×K	859.44	Joback Method
dvisc	0.0027998	Pa×s	360.78	Joback Method
dvisc	0.0014679	Pa×s	398.95	Joback Method

dvisc	0.0008615	Pa×s	437.12	Joback Method
dvisc	0.0005508	Pa×s	475.29	Joback Method
dvisc	0.0003763	Pa×s	513.47	Joback Method
dvisc	0.0002711	Pa×s	551.64	Joback Method
dvisc	0.0002037	Pa×s	589.81	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C706934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume